Dynamics of two interacting electrons in a one-dimensional crystal with impurities

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We investigated the role that the electron-electron interaction plays on the propagating properties of wave packets in a one-dimensional crystal with impurities. We considered two interacting particles with opposite spins in a band, where we treated their interaction along the Hubbard model. We have obtained the density of states of the crystal for different values of the interaction term, as well as solved the dynamical Schrödinger equation by varying the initial conditions. We have introduced a method through which we were able to follow the time evolution of the wave packets for both spins showed in three-dimensional plots, and have evaluated, for each particle, the corresponding $MSD's$ and the centroids as function of time . These measurements allow us to determine the influence of the interaction on dynamical properties. We discussed the combined effect that the extension of the initial wave packets and the interaction strength have on propagating properties. Under certain conditions we obtained an entanglement of the two packets associated with both spins that takes place in a small region of the lattice.

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I. INTRODUCTION

According to the scaling theory of localization developed by Abrahams et al[1] in low dimensional systems (one and two dimensions), any degree of disorder will prevent the appearance of a metallic phase. Moreover, former experiments done with two-dimensional electron systems fabricated on semiconductor surfaces showed a logarithmic increase of resistivity while lowering the temperature[2,3,4,5]. This behavior lends support to the scaling theory of localization, since this happens in case of a weak electron-electron interaction. These results were in agreement with theoretical predictions[6] that *weak* electron-electron interaction increases localization. The above experiments were done with samples of high density of electrons, i.e. systems for which the associated Wigner radius $r_s \ll 1$, which is the ratio between the Coulomb energy to Fermi energy.

However, such a scaling theory does not take into account the electron-electron interaction which was lately believed to be responsible for a metal-insulator transition, observed in several experiments performed at zero magnetic field described below. In the metallic phase, one observes a strong temperature dependence (a steep $d\varrho/dT > 0$) caused by the delocalizing effects produced by the interaction between the particles.

As the density is reduced such that $r_s \gg 1$, the interaction becomes dominant, for that regime Finkelstein[7] and Castellani et al.[8] predicted that for sufficient strong interactions, a 2D system should present a conducting phase as the temperature is lowered. Since recently was possible the fabrication of 2D samples of high quality with very small amount of randomness, measurements were done at very low particles densities. In this way the strongly interacting regime ($r_s \gg 1$) has become experimentally accessible. For instance for $r_s > 10$ experiments done on low-disordered $2D$ silicon samples demonstrated that with increasing electron density one can cross from the insulating regime where the resistance *diverges* with decreasing temperature, to a regime where the resistance *decreases* strongly with decreasing temperature, clearly showing metallic behavior[9,10,11].

In addition to that, in an extensive numerical analysis of the two-dimensional Anderson model with dimerised disorder, we have reported the existence of several dynamical regimes[13,14].

As far as we are concerned there is no a theoretical explanation that describes adequately the metal-insulator transition in two-dimensional systems, as well as the dramatic increase of the spin susceptibility in its vicinity. Comprehensive studies of the state of the art of this intriguing problem are presented by Abrahams et al.[15] and Kravchenko and Sarachik[16].

In one-dimensional systems with random disorder of any intensity, all states are exponentially localized as shown in the pioneering work by Anderson[17] in dealing with diagonal disorder, i.e., a model where the on-site energies are randomly distributed. On the other hand, when some correlation is included in the model, and without considering interaction between particles, this picture is substantially modified, given place to the appearance of extended states and, consequently, carriers are able to propagate through the system. Several structures with correlated disorder show vanishing of localization, when one considers nearest neighbors hopping. Among them one can quote the random-dimer model that can explain the high conductivity of polymers[18,19,20,21]. Another example that show correlated disorder, responsible for particle diffusion in $1D$ is provided by the structures where the on-site energies follow the Fibonacci and Thue-Morse sequences[22,23,24,25,26]. One should mention also the Harper model of a quasicrystal which presents a

mobility edge when the strength of the potential equals the half-bandwidth. Starting with a well localized particle in the lattice, as long as the Harper potential is less than half-bandwidth, we encounter ballistic propagation [27,28,29,30]. The purpose of this work is to analyze the role the electron-electron interaction plays on propagation in some 1D nonperiodic structures. First we present in Sec. II the model assumed for the interaction between two particles in a band, namely the Hubbard Hamiltonian. The two electrons are assumed in the singlet state in order to detect the effect of the Hubbard term, since it acts on opposite spins. We show the density of states for different strengths of the interaction. The dynamics tools introduced in order to characterize the dynamical behavior are presented in Sec. III, namely, the time evolution of the mean square displacement (MSD) and the centroids associated with each of the particles, as well as the construction of 3D graphs of the wave packets evolution. In sec. IV we discuss the interplay between the strength of the interaction U with the initial wave packet extension. In Sec. V we present the results concerning to a 1D crystal with impurities. In Sec. VI we present the conclusion to which we arrived in this work.

II. THE HUBBARD HAMILTONIAN FOR TWO ELECTRONS INTERACTING IN A BAND

With the aim to study the influence of the Coulomb interaction between carriers in a $1D$ lattice, we treat the electron-electron interaction along the Hubbard model[31] in a crystalline system with impurities. As the experiments show, the electron-electron interaction should modify the behavior of the carriers as obtained in a one particle non-interacting scheme. In our work we introduce two interacting particles in an otherwise empty band. The study of such a problem have deserved a number of interesting works due to the relevant question of what is the role of the interaction between electrons on propagating properties in low dimensional disordered systems[32,33,34,35,36,37,38]. We assume that by solving the present problem one can get a better understanding of the role the interaction plays in real systems.

We consider a one-dimensional lattice of N sites with lattice parameter d, for which the Hubbard Hamiltonian is:

$$H = \sum_{r,s} c^{+}_{r,s} c_{r,s} \gamma_r + V \sum_{r,s} (c^{+}_{r+1,s} c_{r,s} + c.c.) + U \sum_{r} \hat{n}_{r\uparrow} \hat{n}_{r\downarrow} \tag{1}$$

were $\gamma_r = \varepsilon_r + Fedr$, ε_r being the on-site energy, F is the intensity of a dc electric field, $c^{+}_{r,s}(c_{r,s})$ is the Fermi creation (destruction) operator for an electron of spin s at site r, V is the hopping term and $\hat{n}_{r\uparrow}(\hat{n}_{r\downarrow})$ is the number operator for spin up (spin down) at site r. As it was said above, in order to analyze the role the U term plays on the dynamics, we treat the case of electrons with opposite spins, the singlet.

A. Energy spectrum for a crystal

To obtain the energy spectrum for the singlet in an impurity-free 1D lattice, we solve the stationary Schrödinger equation in the Wannier representation where we expand the eigenfunction in terms of the kets $|ns, ms\prime>$ that represent the state with one electron of spin s at site n and the other with spin $s\prime$ at site m:

$$\Phi_E = \sum_{ns,ms'} g(ns, ms'; E) \mid ns, ms' > \tag{2}$$

In the Wannier representation we obtain the following set of equations corresponding to energy E:

$$V\ (g_{n+1,m} + g_{n,m+1} + g_{n-1,m} + g_{n,m-1}) + (\gamma_n + \gamma_m + U\delta_{n,m})\ g_{n,m} = E\, g_{n,m} \tag{3}$$

In this equation the first index refers to a particle with spin *up* and the second for spin *down*. The Wannier amplitudes $g_{n\uparrow,m\downarrow}$do not depend on time. For simplicity we omit the label E in the Wannier amplitudes.

For the crystalline case and without the presence of an electric field, all γ_i can be taken as zero. Introducing the center of mass and relative coordinates in units of the

lattice parameter:

$$R = (n+m)/2; \qquad r = n-m \tag{4}$$

and following Hubbard we expand the Wannier amplitudes:

$$g_{n,m} = \sum_{K,k} \Phi(K,k)\ e^{iKR} e^{ikr} \tag{5}$$

to obtain the following equation for the $\Phi(K,k)$:

$$\Phi(K,k) = \frac{\frac{U}{N}\ \sum_{k'} \Phi(K,k')}{E - 2V\cos(\frac{K}{2}+k) - 2V\cos(\frac{K}{2}-k)} \tag{6}$$

which in turn becomes:

$$1 = \frac{U}{N} \sum_{k} \frac{1}{E - \varepsilon_{\frac{K}{2}+k} - \varepsilon_{\frac{K}{2}-k}} \tag{7}$$

For every K we obtain $N-1$ roots of this equation inside the infinities of the right hand side for which $E = \varepsilon_{\frac{K}{2}+k} + \varepsilon_{\frac{K}{2}-k} = 4V\cos\frac{K}{2}\cos k$. At the same time, and provided U is large enough, there appears an extra root outside the band. In this case, by varying K we get an excited second band. By looking at the eigenvalue equation (3) we note its close resemblance with the corresponding Schrödinger equation for *one* particle in a tight-binding $2D$ Hamiltonian, except for the U Hubbard term[39]. The obtained density of states for the crystalline case for $U = 5V$ shown in Fig. 1.a, present two bands. The lower band is very similar to the case of one electron in $2D$ for the reasons stated above and, the excited band has the typical structure of tight-binding $1D$ bands. Moreover, by looking at the equation (7) one notes that $E = U$ is a root of it, which happens for $K = \pm\pi$. This way if U is less than $4V$ we obtain resonant states inside the band, instead of an excited band separated from the $2D$ band for a $U-4V$ gap, that appears when U is greater than $4V$, since the bottom of the excited band occurs at $E = U$. See Fig. 1.b. We conclude that the inclusion of the electron-electron interaction in a crystalline structure in $1D$ have produced a band with a structure similar to a $2D$ band for *one* electron, plus an extra band provided U is great enough.

III. THE DYNAMICS

We follow the time evolution of wave packets in a $1D$ lattice, by assuming the following expansion for the wave function in the Wannier representation

$$\mid \Psi(t) > = \sum_{ns,ms'} f_{ns,ms'}(t)\ \mid ns, ms' > \tag{8}$$

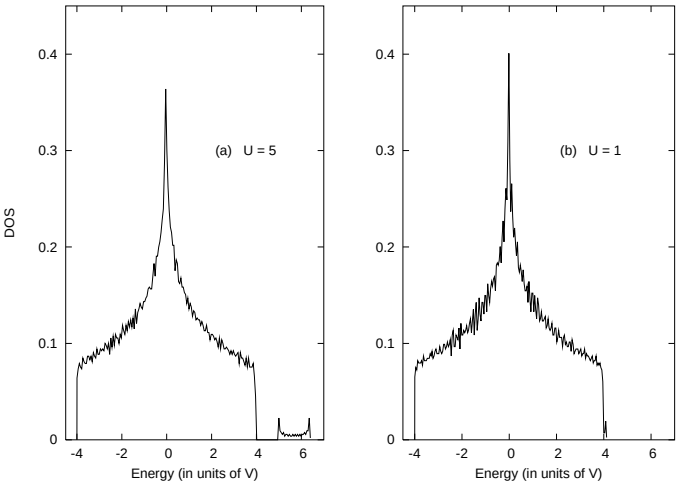

FIG. 1: The density of states in a crystal for: a) $U = 5$, and b) $U = 1$. The energy is in units of the hopping parameter V.

where the Wannier amplitudes now depend on time. The time evolution of the wave function

$$i\hbar\ \frac{\partial \mid \Psi >}{\partial t}\ = H \mid \Psi > \tag{9}$$

becomes in the Wannier representation:

$$i\hbar\ \frac{df_{n,m}}{dt}\ = V\ (f_{n+1,m} + f_{n,m+1} + f_{n-1,m} + f_{n,m-1})\ +\ (\gamma_n + \gamma_m + U\delta_{n,m})\ f_{n,m} \tag{10}$$

We assume the initial condition with an electron around site p with spin *up* and the other around site q with spin *down*. In order to do this, we shall consider the initial condition described by gaussian packets of different standard deviations centered at sites p and q:

$$\mid \Psi(t=0) > = \mid \mathbf{p}_\uparrow, \mathbf{q}_\downarrow > \tag{11}$$

where

$$< n \mid \mathbf{p}_{\uparrow}(0) >= C \exp\left[-\frac{(n-p)^2}{2\sigma^2}\right] \qquad (12)$$

$$< m \mid \mathbf{q}_{\downarrow}(0) >= C \exp\left[-\frac{(m-q)^2}{2\sigma^2}\right] \qquad (13)$$

and C is a normalization constant.

As said before, all γ_i can be taken as zero for the crystalline case without an electric field. We shall consider gaussians with standard deviations σ. The case $\sigma = 0$ corresponds to a particle localized in a single site. In the crystalline case where all ε_n are the same and not taking into account the Hubbard electron-electron interaction, both particles should propagate ballistically in the regular lattice[39]. But now, in the presence of the on-site interaction U, a different behavior should take place. To follow the evolution of the particles injected around sites p and q with spins up and down respectively, we perform the following. We define the mean-square displacement of each electron as indicated below.

$$MSD_{p\uparrow} = \sum_n (n-p)^2 \sum_m \mid f_{n,m}(t) \mid^2 \qquad (14)$$

and

$$MSD_{q\downarrow} = \sum_m (m-q)^2 \sum_n \mid f_{n,m}(t) \mid^2 \qquad (15)$$

At the same time we can follow the centroid of the wave packet associated with the movement of each electron as follows:

$$< \Delta x(t) >_{p\uparrow} = \sum_n (n-p) \sum_m \mid f_{n,m}(t) \mid^2 \qquad (16)$$

and

$$< \Delta x(t) >_{q\downarrow} = \sum_m (m-q) \sum_n \mid f_{n,m}(t) \mid^2 \qquad (17)$$

which will give us the amount of the displacement from the initial positions for both electrons.

At the same time, by taking the absolute value of the difference between the respective centroid positions, we can determine the time evolution of the mean distance of the two electrons, or the size of the propagating pair: $d(t) = | < x(t) >_{p\uparrow} - < x(t) >_{q\downarrow} |$.

In what follows we shall define the energies in units of the hopping parameter V, and the time in dimensionless units $\tau = Vt/\hbar$.

IV. INTERPLAY BETWEEN U AND THE INITIAL WAVE PACKET EXTENSION FOR A CRYSTALLINE CASE

In order to study the combined effect that the interaction and the extension of the initial wave packet have on the propagating properties, we shall analyze the behavior of the MSD's as function of time. We consider the case in which both particles are injected at $t = 0$ in the same position in the lattice. By taking four different initial waves associated with $\sigma = 0$, 1, 2 and 3 we note ballistic propagation in all cases, i.e., $MSD = Dt^2 + C$. In Fig. 2 we have plotted the ballistic coefficient D as function of the interacting Hubbard term U.

We treat first the case of non-interacting electrons, i.e., $U = 0$. We note that the MSD's values decrease when the extension of the initial packets increase. The broader the packet the more inertia it has, it becomes more "massive".

We consider now the interacting case. First, we concentrate on the $\sigma = 0$ case and vary the strength of the Hubbard potential. The U term acts as an on-site energy so that by increasing it, we introduce a barrier that inhibits hopping, the more so, the bigger U is. We still have propagation but with smaller MSD's values as we increase U. The ballistic coefficient D is a monotonically decreasing function of U.

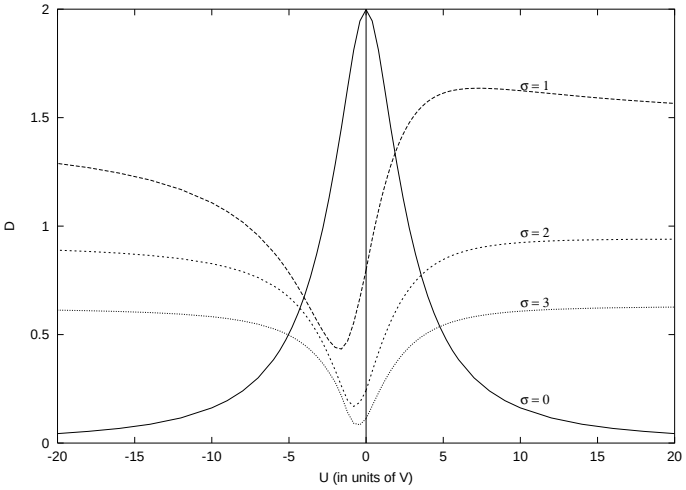

FIG. 2: The MSD coefficient D as function of the interaction U for four cases of initial wave packets: $\sigma = 0$, 1, 2 and 3. As said in the text $MSD/, = /, D/, t^2 + C$

An interesting situation occurs when the initial wave packet has an extension, i.e., $\sigma \neq 0$. At this point we should state that the hopping parameter was assumed to be negative. By looking at the dynamical equation (10) we realize that what is relevant in analyzing propagation is the difference U - V, which can be considered like an effective interaction. This way, when both magnitudes have the same sign the interaction is reduced, while when they have different sign the effective inter-

action is increased. Consider first the case $U > 0$. We obtain in all cases studied ($\sigma = 1$, 2 and 3) the D coefficient increases rapidly with U until reaching a plateau while $D(\sigma_1) > D(\sigma_2) > D(\sigma_3)$, i.e., the more extended the initial wave packet, the more massive it is. This also happens for the non interacting case $U = 0$, as shown above.

Now for $U < 0$ a different behavior is observed, where in this case the effective interaction is reduced. First we take $\sigma = 1$ and see that for $U = -1$ *smaller* values than for $U = 0$ are obtained, while for U= -2 we get even smaller values than for $U = -1$. From then on the MSD's increase monotonically with $\mid U \mid$, such that from $\mid U \mid =$ 5 on, the values are greater than the corresponding to $U = 0$. The minimum of the coefficient D occurs for $U = -1.5$. Taking a more extended initial wave packet, $\sigma = 2$, the same trend is observed, but now the minimum is at $U = -0.75$. Already for $U = -2$ the MSD is larger than for $U = 0$, and from then on they increase monotonically with $\mid U \mid$, as it happens for $\sigma = 1$. As for $\sigma = 3$ it shows the same behavior with the minimum closer to U = 0.

We will explain now the initial decreasing trend for small $\mid U \mid$, when the initial packet has extension different from zero and hopping and interaction parameters have same sign. We have two competing effects to consider, on one side the extension of the packet implies more inertia (smaller MSD values) as said above, on the other hand, the presence of the U repulsive term acts on the different components of the wave trying to push the packet further away. For small $\mid U \mid$, the first effect overcome so one gets smaller MSD values but, increasing $\mid U \mid$, the repulsion dominates so greater values are obtained. Finally, we note a cross over region that happens for $4 < \mid U \mid < 5$, where for the three cases considered: $\sigma = 1$, 2 and 3, the corresponding MSD values are greater than the ones for $\sigma = 0$, for $\mid U \mid \gtrsim 5$.

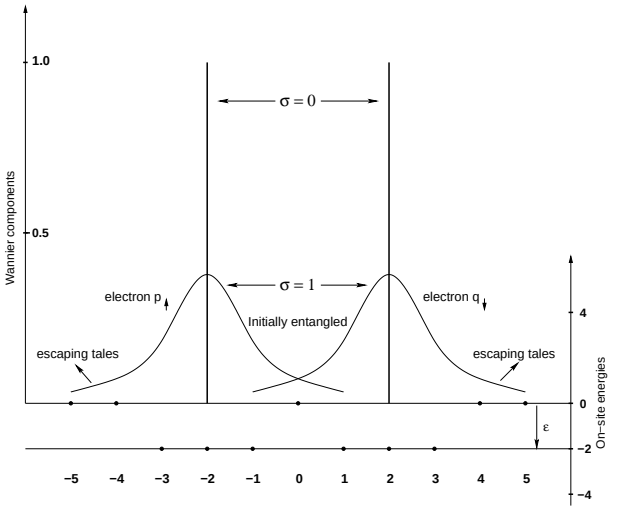

FIG. 3: The initial wave packets for the two configurations assumed: well localized ($\sigma = 0$) and extended ($\sigma = 1$).

V. TWO ELECTRONS IN A CRYSTAL WITH IMPURITIES

We shall consider injected particles at time zero around sites p and q, where these sites as well as their nearest neighbors are taken as impurity levels in an otherwise regular lattice. In Fig. 3, we show the initial wave packets for the configurations $\sigma = 0$ and 1. We illustrate the cases in which the packets are centered at positions ± 2, and the impurity levels at $\varepsilon = -2$, see Fig. 3. Note that for the case $\sigma = 1$ the initial wave packets overlap due to the vicinity of the sites p and q. Obviously for $\sigma = 0$ no overlap is obtained.

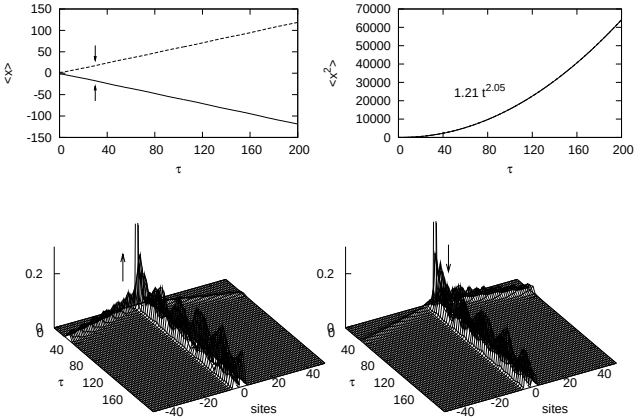

FIG. 4: Show for $\varepsilon = -2V$, $U = 4$ and $\sigma = 0$, in the upper part, the centroids and the MSD as functions of time and in the lower part the time evolution of the up and down spin wave packets. Note that a considerable amount of both waves get trapped around the starting positions, while the rest propagate rapidly given rise to the observed superballistic behavior.

First we assumed the impurity energy levels at $\varepsilon = -2$ and varied σ as well as the interacting factor U. We shall discuss the results for the initially well localized wave packets ($\sigma = 0$) and moderate interaction, $U = 4$, see fig. 4. The centroids clearly start to depart from each other as soon as the up and down packets overlap due to the interaction. The MSD shows a superballistic behavior: Ct^{α} with a time exponent $\alpha = 2.05$. One notes by looking at the wave packets evolution that rather big components of the two waves get trapped around the starting positions due to the well depth. At the same time, the tails of the initial packets are able to propagate, being responsible for the superballistic behavior.

Now by taken $\sigma = 1$ we obtain a completely different picture, we observe an oscillatory movement of the centroids, see Fig. 5. The wave corresponding to each of the particles get trapped in a very small region and one notices that they strongly overlap in such a way that when one is moving to the right the other perform a displacement to the left and vice versa. The up and down spin wave packets get entangled with each other. The trap-

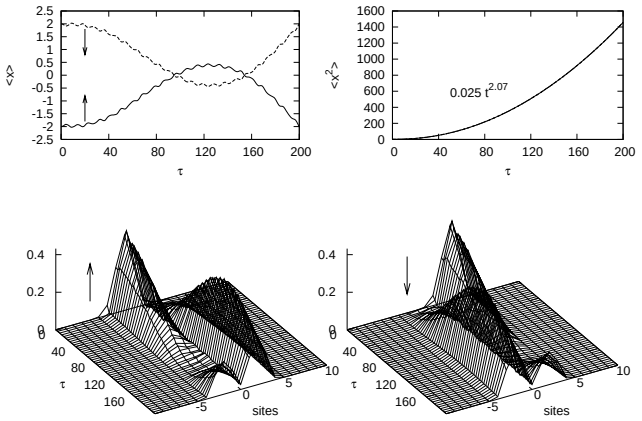

FIG. 5: The same as in Fig. 4 but for $\varepsilon = -2V$, $U = 4$ and $\sigma = 1$. In this case the more extended initial wave packets overlap given rise as a result to an entanglement of the two particles that perform oscillatory movements as time goes. Note that the MSD values are much smaller than in the previous case $\sigma = 0$.

ping of the wave packets can be understood by noticing that the sites covered by the gaussians are degenerate with on-site energies very different from the rest of the lattice, thus inhibiting hopping to distant sites. The behavior of the MSD's proportional to t^2 is due to the escaping of the tails of the initial wave packets that can hop to the near degenerate sites. This case serve to indicate that the propagating properties can not be inferred only from the MSD. In this connection we resort to 3D graphs that show the way the packets evolve in time.

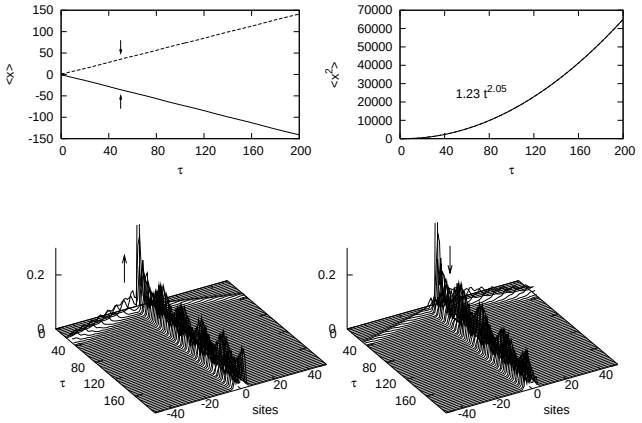

FIG. 6: The same as in Fig. 4 but for $\varepsilon = -2V$, $U = 8$ and $\sigma = 0$

.

Increasing the interaction factor to $U = 8$ and taken $\sigma = 0$ we obtain a similar behavior than the one described above for $U = 4$, see Fig. 6. For the same U and $\sigma = 1$ we observe the same entanglement that occurs for $U = 4$, with the difference that the period of the oscillation of

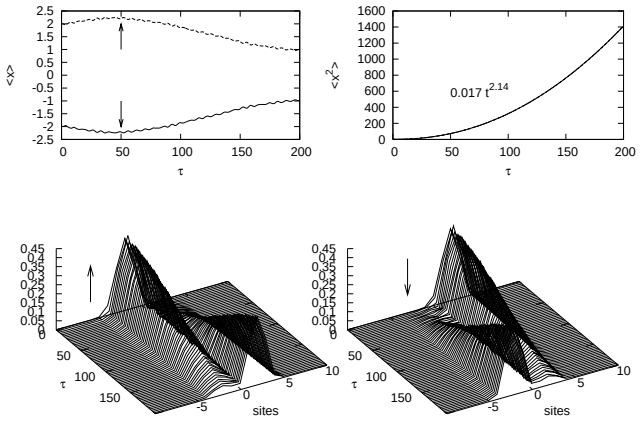

FIG. 7: The same as in Fig. 4 but for $\varepsilon = -2V$, $U = 8$ and $\sigma = 1$. Note the analogous behavior as the shown in the case for $U = 4$.

the centroids is larger in the present case, see Fig. 7.

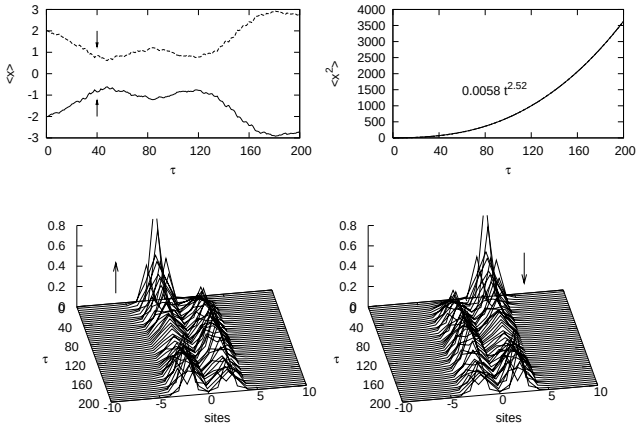

FIG. 8: The same as in Fig. 4 but for $\varepsilon = -4V$, $U = 4$ and $\sigma = 0$.

We treat now the case in which the impurity levels are deeper, i.e., at $\varepsilon = -4$. For the initially well localized packets, $\sigma = 0$, and the interaction $U = 4$, we note that the centroids tend to get near to each other until they fill the repulsion, but they do not depart very much and later on they repeat the tendency to get closer. As for the MSD's the values are much smaller than the corresponding for $\varepsilon = -2$. By looking at the evolution of the wave packets in the 3D graphs it is evident that the packets get trapped due to the deepness of the wells, see Fig. 8. Considering now more extended initial wave packets, $\sigma = 1$, we note that the centroids depart from each other, the MSD's show ballistic behavior due to the escaping tales of the initial wave packets. As for the time evolution of the up and down wave functions we observe that they get trapped around the starting positions. A small amount of the amplitude of each of the up and down waves show a tendency to overlap with the other, see Fig. 9.

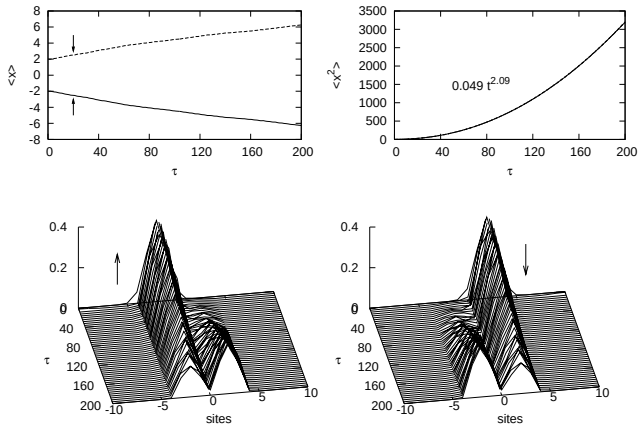

FIG. 9: The same as in Fig. 4 but for $\varepsilon = -4V$, $U = 4$ and $\sigma = 1$.

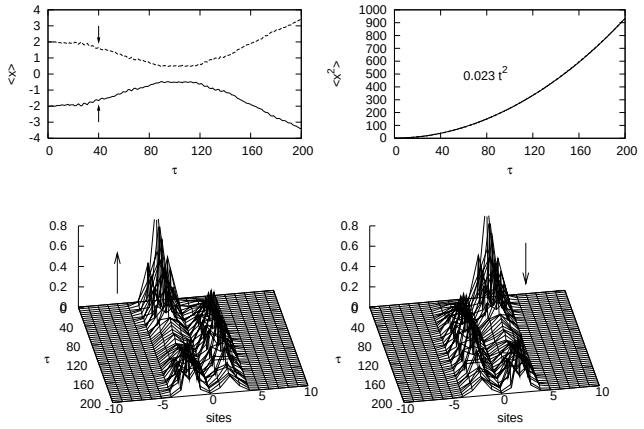

FIG. 10: The same as in Fig. 4 but for$\varepsilon = -4V$, $U = 8$ and $\sigma = 0$.

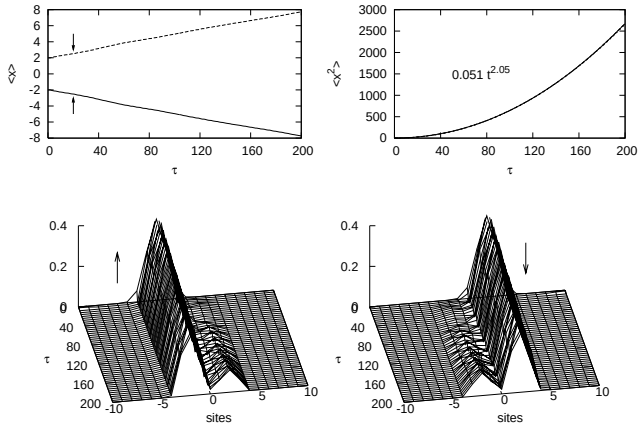

FIG. 11: The same as in Fig. 4 but for$\varepsilon = -4V$, $U = 8$ and $\sigma = 1$.

Now for a strong interaction, $U = 8$ and taken $\sigma = 0$, we observe that the centroids tend to approximate while the MSD's values are much smaller than the corresponding to $\varepsilon = -2$. Due to the deeper impurities levels, the packets get trapped in a very small region of the lattice, see Fig. 10. When we take more extended initial packets, i.e., $\sigma = 1$, the centroids tend to depart from each other, the MSD's are larger than the corresponding to the former case, $\sigma = 0$, and the wave packets perform the same kind of oscillations, see Fig. 11.

The time limit taken in our calculation was 10^{-11}sec, longer than any reasonable collision time, this implies that in order to avoid undesirable boundary effects, we have included lattices up to 1000 sites. We used the Runge-Kutta method to integrate the equations of motion.

VI. CONCLUSIONS

In this work we analyzed the role the electron-electron interaction plays in one-dimensional disordered systems, in particular, a crystalline lattice with impurities. Two electrons with opposite spins were introduced in a band where their interaction was assumed along the Hubbard model. We have obtained the energy spectrum of a crystal considering different values of the interaction strength. The obtained density of states show that for sufficiently large U, two bands are present separated by a gap of intensity $U - 4V$. The lower band has the feature of the one corresponding to a single particle in a 2D crystal, while the excited band has the structure of a 1D tight-binding crystal.

As for the dynamical properties, we analyzed the interplay between the initial wave packet extensions and, for both, positive and negative values of the interaction U.

In the non-interacting case, $U = 0$, we show that by increasing the extension of the packets, one reduces the MSD values, the more so, the more extended the initial wave packets, they become more "massive".

In the case of a positive U, the obtained MSD increases rapidly from the non interacting case $U = 0$. For negative U, a different initial behavior is observed. As U is near the origin the MSD decrease until a minimum value is achieved, and from then on it increases reaching a plateau. For both the positive and negative values of U there exists a cross over region as explained in the text.

Next we analyze the propagation that takes place when we introduce the two interacting particles at impurity sites in an otherwise periodic crystal. We have encountered situations for which the MSD as function of time presents superballistic behavior, although when looking at the packet we realize that most of it get trapped in a small region of the lattice. That is why the propagating properties can not be inferred from the MSD alone. When we consider moderate impurity levels, in our case $\varepsilon = -2V$, the response of the system with regard to the

initial conditions are very different. In fact, when we start with very well localized particles, $\sigma = 0$, the centroids depart from each other for every intensity of the interaction, while for the less localized initial packets, $\sigma = 1$, the two particles get entangled, trapped in the impurity region, we observe the centroids performing a periodic movement. When considering deeper impurity levels such as $\varepsilon = -4$ no matter what the extension of the initial waves packets are, the result indicate that the particles remain localized around the starting positions, this is true for every interaction strength.

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